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It is my pleasure to dedicate this paper to my dear friend and mentor Prof. Leonid Slepyan.

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Internal resonances and relaxation memory kernels in composites

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In heterogeneous composite materials, the behaviour of the medium on larger scales is determined by the microgeometry and properties of the constituents on finer scales. To model the influence of the microlevel processes in composite materials, they are described as materials with memory in which the constitutive relations between stress and strain are given as time-domain convolutions with some relaxation kernel. The paper reveals the relationship between the viscoelastic relaxation kernel and the spectral measure in the Stieltjes integral representation of the effective properties of composites. This spectral measure contains all information about the microgeometry of the material, thus providing a link between the relaxation kernel and the microstructure of the composite. We show that the internal resonances of the microstructure determine the characteristic relaxation times of the fading memory kernel and can be used to introduce a set of internal variables that captures dissipation at the microscale.

This article is part of the theme issue 'Modelling of dynamic phenomena and localization in structured media (part 2)'.

1. Introduction

Multiscale hierarchical composite materials exhibit different types of behaviour on different scales with the finest scales determining the properties of the constituents on larger scales. Viscoelastic properties of materials are the result of dissipative processes on fine scales which could stem from nonlinear wave energy dissipation [1–3] in atomic lattices, from grain boundaries dislocations in thin films and polycrystalline materials [4,5], from damage, fracturing and repairing at the microscale in polymers and biological materials [6].

The wave propagating through a composite medium excites microlevel processes of different characteristic wavelengths and internal scales. At the macroscale, the propagation of time-dependent signals or stresses in such materials is influenced by these microlevel processes and is characterized by frequency dispersion and energy dissipation. In a non-dispersive homogeneous medium, all waves in a packet of waves of different frequencies propagate at the same speed, so that the packet travels without changing its shape. In a medium with microstructure, every wave in the packet experiences multiple scatterings from the boundaries of inclusions or inhomogeneities; this leads to dissipation of the energy of the wave that depends on the particular wavelength. Hence, waves of different frequencies dissipate different amounts of energy and travel at different speeds, this results in changing the shape of the wave packet with time and propagation distance. Due to thermodynamic constraints and Kramers–Kronig relations, these two processes, frequency dispersion and energy dissipation, are necessarily present in all microstructured materials. It is known that the presence of viscoelastic constituents in the composite results in long memory effects in the homogenized material [7]. To model the influence of the microlevel processes in such materials, they are described as materials with memory [8–10] in which the constitutive relations between stress and strain are given as time-domain convolutional relations with some relaxation kernel. These relaxation kernels, often built from the spring and the dashpot building blocks connected in parallel and/or in series, provide phenomenological models that describe the viscoelastic behaviour of many materials [11–13]. However, the relationships between the relaxation kernels and the properties and structure of the medium are not quite known. Revealing the actual relationships between the relaxation function and the structure of the composite is a challenging problem.

In the present paper, we derive an exact relationship between the viscoelastic relaxation memory kernel in composite materials and the spectral measure in the Stieltjes analytic representation of the effective properties. As the spectral measure contains all information about the microgeometry of the material, the derived relationship between the spectral measure and the relaxation function provides a link between the relaxation kernel and the microstructure of the composite. The parameters of a composite's microgeometry are incorporated into the spectral measure in the analytic representation through the n-point correlation functions of the microstructure. We show that the spectral measure and the internal resonances of the microstructure determine the characteristic relaxation times of the fading memory kernel and can be used to introduce a set of internal variables that capture dissipation at the microscale and to derive equations for their evolution.

Stieltjes analytic representation of the effective properties of composite materials is a powerful tool developed in the course of homogenization of electric, transport and elasticity problems for heterogeneous materials [5,14–22]. This integral representation establishes a relation between the effective moduli of a composite and its microgeometry through the spectral measure of a corresponding operator. In particular, the moments of the spectral measure in this representation are linked to the n-point correlation functions of the microstructure. An important characteristic of the Stieltjes representation of the effective properties is that it factors out the dependence on the constituents in the composite from the dependence on the microstructure. The information about the microstructure is contained in the spectral measure in this representation. This feature can be used to solve the inverse homogenization problem [22–24], which requires to recover microstructural information from known effective properties. It was shown that the spectral measure can be uniquely recovered from the measurements of the effective property over a range of frequencies [5,24], however, the problem is ill-posed and needs regularization. Inverse homogenization for viscoelastic composites [22,25] was used to recover bone porosity from simulated measurements of the complex shear modulus. The spectral measure can be numerically calculated using the discretized structure of composites [26]. It was shown that the spectral measure of random composites and the eigenvalue spacing distributions have features similar to the features of the spectra of random matrices [27] and could have a very complex structure.

The idea that the convolution in the viscoelastic constitutive relation may be eliminated by introducing internal or memory variables has been efficiently used in many works in simulations of wave propagation in viscoelastic media [28–33], and in modelling and simulations of effective behaviour of linear viscoelastic composite materials [34–37]. For a linear isotropic viscoelastic material, an existing approach to the internal memory variables in numerical simulations of wave propagation in viscoelastic media [28–33] uses the integral representation of the complex modulus approximated with a low-order rational approximation. This allows transforming the time-domain viscoelastic stress–strain relation into a system of first-order differential equations for the unknown internal variable functions to be solved together with the wave equation of motion in viscoelastic wave-field numerical simulations. The internal variables approach extended to modelling of the relaxation in viscoelastic composite materials [34–37] is based on approximation of the relaxation kernel using the collocation method. The description of the viscoelastic constitutive law using a finite set of internal variables was discussed in [34], where an approximation of the relaxation spectrum was developed. It was noted that this description is exact for Hashin–Shtrikman composite and the analytical expressions for the relaxation parameters were derived. In the case of a continuous relaxation spectrum, the internal variables formulation was considered in [35,37]. In particular cases when a formula for the effective property of the composite is available, discrete approximation of the relaxation kernel can be used to formulate a system of first-order differential equations for the internal variables to be solved at each time step during the evolution of the stress history instead of keeping it in the computer memory.

The current work extends the previous results and relates the relaxation function and the memory kernel to the spectral function of the composite and thus to the structure of the material at the microscale, the results do not rely on any particular microgeometry. In the case when an analytic formula for the effective properties is available, the geometric parameters can be directly related to the relaxation constants in the memory kernel, but even when no analytic formula is known, the spectral measure μ can be numerically calculated as in [26] and used to characterize the relaxation behaviour or to formulate a system of differential equations for the internal variables. We show that the coefficients of the system of the differential equations can be derived from poles and residues of the Padé approximant of the spectral measure. We show that the internal resonances dependent on the microstructure of the composite determine the relaxation times of the memory kernel as well as equations for the evolution of internal memory variables characterizing dispersion and dissipation in a wave propagating through the composite material.

The outline of the paper is as follows. A short introduction to the viscoelastic problem is presented in §2. Then, in §3, we develop the Stieltjes analytic representation of the effective properties of a composite made of two materials. We assume further that one of the materials is viscoelastic described by the basic Maxwell model, and the second material is elastic. A general relation between the spectral measure in the analytic representation and the relaxation function is derived in §4. We also find the effective relaxation function and parameters of the relaxation kernel for several composites' microgeometries using corresponding spectral measures. A brief summary of results concerning the Padé approximation is presented in §5. In §6, we show how parameters of the effective relaxation kernel and poles and residues of the Padé approximation of the spectral function determine equations for the evolution of the internal memory variables in application to simulation of waves propagation in viscoelastic media.

2. Viscoelastic convolutional stress–strain relation in time domain

We consider a time-domain equation of motion for a scalar potential as a model for a plane compressional or shear wave propagating in a homogeneous isotropic linear viscoelastic medium

$$\varrho \frac{\partial^2 u}{\partial t^2} = \nabla \cdot \sigma . \tag{2.1}$$

Here, $u(x,t)$ is the displacement, ϱ is the mass density and $\sigma(x,t)$ is the time-dependent stress which is related to the strain $\varepsilon = \nabla u$ with a convolutional in time constitutive relation. We consider equation (2.1) to be a result of homogenization of a microscale problem in which the coefficients in the equation are spatially oscillating functions changing on a very fine scale. This corresponds to the waves propagating in composite materials and materials with microstructure.

Based on the Boltzman principle, the relationship between the time-dependent stress σ and the time-dependent strain rate $\dot{\varepsilon}$ is represented in viscoelasticity as a convolution of the strain rate with the relaxation function ψ, which provides a generalization of Hooke's law applicable to viscoelastic materials.

$$\sigma = \psi * \partial_t \varepsilon = \int_{-\infty}^{t} \psi(t-\tau)\,\mathrm{d}\varepsilon(\tau). \tag{2.2}$$

The relaxation function characterizes the fading memory effects in the material and is determined by characteristic relaxation times or relaxation constants. We will show later that these relaxation times are related to the internal scales in the composite.

Taking the Fourier transform of the convolution

$$\sigma = \partial_t \psi * \varepsilon, \tag{2.3}$$

we have the relationship between the stress and strain in the frequency domain $\sigma(\omega) = M(\omega)\varepsilon(\omega)$, where $M(\omega)$ is the complex viscoelastic modulus and ω is the frequency. We use the same notation σ and ε for stress and strain in both time and frequency domains as this should not cause any confusion. The complex viscoelastic modulus $M(\omega)$ is given as

$$M(\omega) = \mathcal{F}\{\partial_t \psi\}(\omega) = \int_{-\infty}^{\infty} \partial_t \psi(t) \exp(-\mathrm{i}\omega t)\,\mathrm{d}t. \tag{2.4}$$

It is assumed that the relaxation function of the medium $\psi(t)$ is zero for $t < 0$, so that it can be represented as

$$\psi(t) = \hat{\psi}(t)H(t) \quad \text{and} \quad \partial_t \psi(t) = \hat{\psi}(0)\delta(t) + \partial_t \hat{\psi}(t)H(t) \tag{2.5}$$

for some function $\hat{\psi}(t)$; here $H(t)$ is the Heaviside function. Using this representation the function $M(\omega)$ can be written as

$$M(\omega) = \psi(0^+) + \int_{0}^{\infty} \partial_t \psi(t) \exp(-\mathrm{i}\omega t)\,\mathrm{d}t. \tag{2.6}$$

Using the constitutive relation between the stress σ and strain ε in the frequency domain, the complex velocity and the quality factor Q in an attenuating medium are given as [12]

$$V(\omega) = \left(\frac{M(\omega)}{\varrho}\right)^{1/2} \quad \text{and} \quad \mathrm{Q}(\omega) = \frac{\operatorname{Re} M(\omega)}{\operatorname{Im} M(\omega)}. \tag{2.7}$$

The dimensionless quality factor Q, uniquely determined by $M(\omega)$, and its reciprocal $\mathrm{Q}^{-1}(\omega)$ representing the internal friction, are often used for evaluation of the absorption, attenuation and dissipation of the waves in engineering, materials and geophysical applications.

To discuss the time-dependent stress and strain in viscoelastic materials, we consider one of the most general relationships that relates the derivatives of the stress and strain as

$$\sum_{k=0}^{m} a_k \frac{\mathrm{d}^k}{\mathrm{d}t^k}\sigma = \sum_{k=0}^{n} b_k \frac{\mathrm{d}^k}{\mathrm{d}t^k}\varepsilon. \tag{2.8}$$

Taking the Fourier transform, we have a representation of the viscoelastic modulus on the complex plane as a quotient of two polynomials $Q(\mathrm{i}\omega)$ and $P(\mathrm{i}\omega)$ with coefficients b_k, a_k and the roots α_k^{ϵ} and α_k^{σ}:

$$\sigma(i\omega) = \frac{Q(\mathrm{i}\omega)}{P(\mathrm{i}\omega)}\varepsilon(\mathrm{i}\omega) = \sum_k \frac{Q(\alpha_k^{\sigma})}{P'(\alpha_k^{\sigma})(\mathrm{i}\omega - \alpha_k^{\sigma})}\varepsilon(\mathrm{i}\omega). \tag{2.9}$$

Here, the last equality is obtained by using the Lagrange interpolation formula and expanding the quotient of polynomials in terms of partial fractions. The time-domain series (Prony series) is obtained by taking the Fourier (or Laplace with $s = \mathrm{i}\omega$) transform

$$M(t) = \sum_k M_k \exp(\alpha_k^\sigma t) \quad \text{and} \quad M_k = \frac{Q(\alpha_k^\sigma)}{P'(\alpha_k^\sigma)}. \tag{2.10}$$

Taking into account the behaviour of the viscoelastic modulus at time equal to zero and infinity, these series are often put into the form

$$M(t) = M_\mathrm{R} + \sum_{i=1}^{N} M_i \exp\left(-\frac{t}{\tau_i}\right) = M_\mathrm{U} - \sum_{i=1}^{N} M_i \left[1 - \exp\left(-\frac{t}{\tau_i}\right)\right], \tag{2.11}$$

where τ_i are the relaxation times of the medium, M_R is the relaxed modulus at $t = \infty$, M_U is the unrelaxed modulus at $t = 0$ and their difference δM is the relaxation of the modulus, $\delta M = M_\mathrm{U} - M_\mathrm{R}$. The relaxed M_R and unrelaxed M_U moduli can be obtained using corresponding asymptotics in frequency as

$$M_\mathrm{U} = \lim_{\omega \to \infty} M(\omega), \quad M_\mathrm{R} = \lim_{\omega \to 0} M(\omega) \quad \text{with } \delta M = \sum_{i=1}^{N} M_i = M_\mathrm{U} - M_\mathrm{R}, \tag{2.12}$$

so that the relaxed modulus $M_\mathrm{R} \geq 0$ is an equilibrium modulus corresponding to a very long time ($t \to \infty$, $\omega \to 0$, with $M_\mathrm{R} = 0$ for viscoelastic fluids), and the unrelaxed modulus $M_\mathrm{U} > 0$ is an elastic modulus corresponding to the instantaneous response of material ($t \to 0$, $\omega \to \infty$).

Finally, in the case of a continuous relaxation spectrum, the viscoelastic modulus in the frequency domain can be expressed as

$$M(\omega) = M_\mathrm{U} - \delta M \int_0^\infty \frac{\mathrm{d}\eta(x)}{\mathrm{i}\omega + x}, \tag{2.13}$$

where $x^{-1} = \tau$ is the relaxation time and $\mathrm{d}\eta(x) = \hat{\Phi}(x)\,\mathrm{d}x$ or $\mathrm{d}\eta(x) = \Phi(-\ln\tau)\,\mathrm{d}x$, and the non-negative distribution Φ is the normalized relaxation spectrum of the medium.

3. Spectral representation of the effective property

On a microscale, we consider a random or periodic two-phase composite with the values of the parameters c_1 in the region Ω_1 and c_2 in the region Ω_2. To describe the geometry of the regions Ω_1 and Ω_2, we introduce the characteristic function $\chi = \chi(x)$ of domain Ω_1. The function $\chi(x)$ takes value 1 if $x \in \Omega_1$ and zero if $x \in \Omega_2$

$$\chi(x) = \begin{cases} 1 & \text{if } x \in \Omega_1, \\ 0 & \text{otherwise.} \end{cases} \tag{3.1}$$

Then, the material property of the medium is $c(x)$,

$$c(x) = c_1 \chi(x) + c_2(1 - \chi(x)). \tag{3.2}$$

We assume that the scale of variation of the microstructure is much smaller than the wavelengths of the effective displacement u in (2.1), then

$$\nabla \cdot (c_1 \chi(x) + c_2(1 - \chi(x)))\varepsilon = 0. \tag{3.3}$$

The last expression can be brought to the form

$$\nabla \cdot \chi\varepsilon = s\nabla \cdot \varepsilon \quad \text{where} \quad s = \frac{1}{1 - c_1/c_2}. \tag{3.4}$$

Let $\nabla\phi$ be a mean zero perturbation of the constant field e_k , so that $\varepsilon = e_k + \nabla\phi$. Then,

$$\nabla \cdot \chi(\nabla\phi + e_k) = s\Delta\phi, \tag{3.5}$$

where $(-\Delta)$ is the Laplace operator, and

$$(\nabla\phi + e_k) + \frac{1}{s}\nabla(-\Delta)^{-1}\nabla\cdot\chi(\nabla\phi + e_k) = e_k. \tag{3.6}$$

Let $\Gamma = \nabla(-\Delta)^{-1}(\nabla\cdot)$, so that Γ is an operator projecting vector fields onto a subspace of curl-free, zero mean fields. Then,

$$\varepsilon = s(sI + \Gamma\chi)^{-1}e_k. \tag{3.7}$$

With the function χ in the inner product, $\Gamma\chi$ is a self-adjoint operator, $\|\Gamma\chi\| \le 1$. Formula (3.7) represents ε as a function of the operator $\Gamma\chi$. Using the spectral resolution of $\Gamma\chi$ with the projection valued measure Q, one can derive the following representation for ε:

$$\varepsilon(s) = \int_0^1 \frac{s}{s-z}\,\mathrm{d}Q(z)\,e_k. \tag{3.8}$$

Next, we obtain the Stieltjes integral representation on the plane of the complex variable s. Consider a function $F(s)$ assuming that c^* is isotropic,

$$F(s) = 1 - \frac{c^*(s)}{c_2} = 1 - \langle (c_1\chi + c_2(1-\chi))\varepsilon, e_k\rangle = \langle s^{-1}\chi\varepsilon, e_k\rangle. \tag{3.9}$$

Using (3.8), we obtain

$$F(s) = \langle \chi(sI + \Gamma\chi)^{-1}e_k, e_k\rangle = \int_0^1 \frac{\langle \chi\,\mathrm{d}Q(z)e_k, e_k\rangle}{s-z}. \tag{3.10}$$

Introduce a function μ corresponding to the spectral measure Q, $\mathrm{d}\mu_{jk}(z) = \langle \chi\,\mathrm{d}Q(z)e_j, e_k\rangle$. We note that generally this measure is a matrix measure, however, assuming the homogenized medium is isotropic, we focus on the diagonal element μ_{kk} which is a positive function of bounded variation. We have now for function $F(s)$

$$F(s) = 1 - \frac{c^*}{c_2} = \int_0^1 \frac{\mathrm{d}\mu(z)}{s-z} \quad \text{and} \quad s = \frac{1}{1 - c_1/c_2}. \tag{3.11}$$

This gives the representation of $F(s)$ as an analytic function on the complex plane of variable s. For a two-phase composite of materials c_1, c_2, the analytic representation for effective c^* separates parameter information in s from information about the microgeometry contained in μ. From (3.11), we have

$$c^* = c_2(1 - F(s)) = c_2 - c_2\int_0^1 \frac{\mathrm{d}\mu(z)}{s-z}. \tag{3.12}$$

Geometric information about the microstructure is incorporated into μ via its moments, which can be calculated from the correlation functions of the medium

$$\mu^n = \int_0^1 z^n\,\mathrm{d}\mu(z) = (-1)^n\langle \chi[(\Gamma\chi)^n e_k]\cdot e_k\rangle. \tag{3.13}$$

In particular, the zeroth moment μ_0 is the volume fraction f of one component in the composite

$$\mu_0 = \int_0^1 \mathrm{d}\mu(z) = \langle\chi\rangle = f. \tag{3.14}$$

The relationships between the composite's microstructure and the spectral measure in the Stieltjes representation (3.11) was a topic of previous investigations in forward and inverse homogenization. The uniqueness of reconstruction of the measure μ was shown in the case when the effective property c^* is known in a range of frequency [24]. The moments of the measure can also be uniquely reconstructed under the same conditions [38], and in particular, the zeroth moment μ_0, which defines the volume fraction of one component in the composite, is uniquely recoverable. The gaps in support of the spectral measure characterize the inclusions separation [39,40].

4. Viscoelastic modulus for a two-phase composite material

Now, we specify the materials in the domain and assume that Ω is filled with a heterogeneous two-phase composite material. We will calculate the effective modulus c^* and the relaxation function ψ^* of such a composite. We assume that the phase occupying a subdomain Ω_1 is a viscoelastic phase with viscoelastic modulus c_1 given by the Maxwell model with parameters M_u (the elastic constant of the spring), η_0 (viscosity of the dashpot), and the relaxation constant $\tau = \eta_0/M_u$. In accordance with (2.8) this model is described by solution of the equation

$$\sigma + \tau\partial_t\sigma = \eta_0\partial_t\epsilon. \tag{4.1}$$

The second phase is isotropic elastic material with the stiffness c_0 in the subdomain Ω_0, and $\Omega = \Omega_1 \cup \Omega_0$.

The relaxation function corresponding to the Maxwell model of the viscoelastic material and its time derivative are

$$\psi(t) = M_u \exp\left(-\frac{t}{\tau}\right) H(t) \quad \text{and} \quad \partial_t\psi = M_u\delta(t) - \frac{M_u}{\tau}\exp\left(-\frac{t}{\tau}\right) H(t). \tag{4.2}$$

The complex viscoelastic modulus c_1 is calculated as

$$\mathcal{F}\{\partial_t\psi\}(\omega) = \int_{-\infty}^{\infty} \partial_t\psi(t)\exp(-\mathrm{i}\omega t)\,\mathrm{d}t. \tag{4.3}$$

Using (4.2),

$$c_1(\omega) = M_u - \frac{M_u}{\tau}\int_0^{\infty} \exp\left(-\frac{t}{\tau}\right)\exp(-\mathrm{i}\omega t)\,\mathrm{d}t = M_u - \frac{M_u}{1+\mathrm{i}\omega\tau}. \tag{4.4}$$

Introduce the complex parameter s which, in this case, is $s = 1/(1 - c_1/c_0)$ and $s = s(\omega)$ as $c_1 = c_1(\omega)$. To simplify the notation, we assume that $M_u = c_0 = 1$. Then, $s = 1 + \mathrm{i}\omega\tau$.

Proposition 4.1. *The relaxation function ψ^* of a composite, made of two materials with properties c_0 and c_1 introduced above, is determined by the spectral measure μ in the Stieltjes spectral representation* (3.11)*:*

$$\psi^*(t) = H(t) + \int_0^1 A^*(z)\,\mathrm{e}^{-t/\tau^*(z)}\,\mathrm{d}\mu(z)\,H(t), \quad A^*(z) = \frac{1}{1-z}\tau, \quad \tau^*(z) = \frac{\tau}{1-z}. \tag{4.5}$$

Indeed, using the Fourier transform we represent $F(s)$ in (3.11) as

$$F(s) = 1 - \frac{c^*}{c_0} = \int_0^1 \frac{\mathrm{d}\mu(z)}{s-z} = \int_0^1 \frac{1}{\tau}\,\mathrm{d}\mu(z)\int_0^{\infty}\exp\left(-t\left[\mathrm{i}\omega + \frac{(1-z)}{\tau}\right]\right)\mathrm{d}t. \tag{4.6}$$

Changing the order of integration in the last integral, we have

$$\int_0^{\infty} \mathrm{e}^{-\mathrm{i}\omega t}\int_0^1 \frac{1}{\tau}\mathrm{e}^{-t(1-z)/\tau}\,\mathrm{d}\mu(z)\,\mathrm{d}t. \tag{4.7}$$

This gives us the time derivative of the relaxation function $\partial_t\psi^*$ of the composite

$$\partial_t\psi^*(t) = \delta(t) - \int_0^1 \frac{1}{\tau}\,\mathrm{e}^{-t(1-z)/\tau}\,\mathrm{d}\mu(z)\,H(t). \tag{4.8}$$

This can be presented as

$$\partial_t\psi^*(t) = \delta(t) - \int_0^1 \frac{A^*(z)}{\tau^*(z)}\,\mathrm{e}^{-t/\tau^*(z)}\,\mathrm{d}\mu(z)\,H(t). \tag{4.9}$$

The relaxation function can now be written in terms of the spectral measure μ:

$$\psi^*(t) = H(t) + \int_0^1 \frac{\mathrm{e}^{-t(1-z)/\tau}}{1-z}\,\mathrm{d}\mu(z)H(t) = H(t) + \int_0^1 A^*(z)\,\mathrm{e}^{-t/\tau^*(z)}\,\mathrm{d}\mu(z)H(t), \tag{4.10}$$

where the parameters $A^*(z)$ and $\tau^*(z)$ of the relaxation function ψ^* as functions of the spectral parameter z in the unit interval are

$$A^*(z) = \frac{1}{1-z} \quad \text{and} \quad \tau^*(z) = \frac{\tau}{1-z}. \tag{4.11}$$

Example 4.2 (One-pole spectrum). Let us consider a composite material for which the spectral representation derived in the previous section reduces to a one-pole representation. An example of such composites are given by the Hashin–Shtrikman coated sphere model, or the materials in which the volume fraction of the viscoelastic phase is small. In this case, the function $F(s)$ in (3.11) takes the form

$$F(s) = 1 - \frac{c^*}{c_0} = \int_0^1 \frac{\mathrm{d}\mu(z)}{s-z} = \frac{m_0}{s-z_0}, \tag{4.12}$$

where the values of m_0 and z_0 are determined by the microgeometry of the composite. We express the effective modulus c^* from (4.12)

$$c^*(\omega) = c_0 - c_0 F(s) = c_0 - c_0 \frac{m_0}{s(\omega) - z_0}. \tag{4.13}$$

Here, $c_0 = 1$ is the elastic modulus of the elastic phase in the composite and does not depend on frequency. Substituting $s(\omega)$ and taking the Fourier transform, we find the derivative of the relaxation function of the composite

$$1 - \frac{m_0}{s(\omega) - z_0} = 1 - \frac{m_0}{\tau} \int_0^\infty \exp\left(-t\left[\frac{(1-z_0)}{\tau} + \mathrm{i}\omega\right]\right) \mathrm{d}t = \mathcal{F}\{\partial_t \psi^*\}(\omega). \tag{4.14}$$

Here, the time derivative of the effective relaxation function $\partial\psi^*$ is

$$\partial_t \psi^* = \delta(t) - \frac{A_1^*}{\tau_1^*} \exp\left(-\frac{t}{\tau_1^*}\right) H(t), \quad A_1^* = \frac{m_0}{(1-z_0)}\tau, \quad \tau_1^* = \frac{\tau}{(1-z_0)} \tag{4.15}$$

and the effective relaxation function ψ^* is

$$\psi^* = H(t) + A_1^* \exp\left(-\frac{t}{\tau_1^*}\right) H(t). \tag{4.16}$$

As expected, the composite is not a viscoelastic fluid but has the elastic modulus as the elastic phase; however, the viscoelastic parameters of the microstructured material differ from the corresponding parameters of the viscoelastic component.

Example 4.3 (Discrete spectrum). Next, we extend the consideration to the case of the spectral function $F(s)$ with n poles in the spectral interval. In this case,

$$F(s) = \int_0^1 \frac{\mathrm{d}\mu(z)}{s-z} = \sum_{k=1}^{n} \frac{m_k}{s-z_k}. \tag{4.17}$$

We deal with the same materials in the composite with properties $c_0 = 1$ and $c_1(\omega)$ given in (4.4) with $M_u = 1$, so that $s = 1 + \mathrm{i}\omega\tau$. Then, from (4.17),

$$F(\omega) = \sum_k \frac{m_k}{\tau} \int_0^\infty \exp\left(-t\left[\mathrm{i}\omega + \frac{(1-z_k)}{\tau}\right]\right) \mathrm{d}t. \tag{4.18}$$

Introducing $\tau_k^* = \tau/(1-z_k)$, we have

$$\partial_t \psi^*(t) = \delta(t) - \sum_k \frac{m_k}{\tau} \exp\left(-\frac{t}{\tau_k^*}\right) H(t), \tag{4.19}$$

This allows us to find the relaxation function ψ^* of the composite

$$\psi^*(t) = H(t) + \sum_k A_k^* \exp\left(-\frac{t}{\tau_k^*}\right) H(t), \tag{4.20}$$

and present the time derivative $\partial_t\psi^*(t)$ in the form

$$\partial_t\psi^*(t) = \delta(t) - \sum_k \frac{A_k^*}{\tau_k^*} \exp\left(-\frac{t}{\tau_k^*}\right) H(t), \tag{4.21}$$

with relaxation parameters A_k^*, τ_k^*

$$A_k^* = \frac{m_k}{1 - z_k} \quad \text{and} \quad \tau_k^* = \frac{\tau}{(1 - z_k)}, \tag{4.22}$$

intrinsically related to the microstructure of the composite material. Hence the internal resonances of the microstructure determine the characteristic relaxation times of the fading memory kernel in (2.2).

Proposition 4.4. *For the same two phases in the composite, the continuous relaxation kernel $\eta(x)$ in (2.13) is determined by the spectral measure in the Stieltjes representation (3.11).*

To show this, we substitute $s = 1 + \mathrm{i}\omega\tau$ and make a change of variables in the integral in (3.11)

$$\int_0^1 \frac{\mathrm{d}\mu(z)}{s - z} = \int_0^1 \frac{\mathrm{d}\mu(z)/\tau}{\mathrm{i}\omega + \frac{1-z}{\tau}}. \tag{4.23}$$

Making a change of variables $x = (1 - z)/\tau$, we end up with the integral in (2.13) with the relaxation kernel $\eta(x)$. Alternatively, one could approximate the measure μ using the Padé approximation and after changing variables, let the number of terms go to infinity.

5. Resonances at the microlevel and the Padé approximation

For composites with a discrete spectrum the spectral function μ describes the resonances in the fine scale problem. For such composites μ has the form

$$\mathrm{d}\mu(z) = \sum_k m_k \delta(z - z_k)\,\mathrm{d}z \quad \text{and} \quad \mu(z) = \sum_k m_k H(z - z_k), \tag{5.1}$$

where $H(z)$ is the Heaviside function. In this case, the poles z_k are the internal resonances generated by the microgeometry of the composite, and the representation for the function $F(s)$ has the form

$$F(s) = \int_0^1 \frac{\mathrm{d}\mu(z)}{s - z} = \sum_k \frac{m_k}{s - z_k}. \tag{5.2}$$

In the case of a continuous function μ, an efficient way to construct a discrete approximation to the spectral function is to use the Padé approximation [41]. The Padé approximation to the scalar spectral function μ was constructed in [42]. In a scalar case, a diagonal Padé approximant of order n to the function $F(s)$ is a unique rational function

$$\pi_n = \frac{Q_n(s)}{P_n(s)} \quad \text{s.t.} \quad P_n(s)F(s) - Q_n(s) = O\left(\frac{1}{s^{n+1}}\right), \tag{5.3}$$

where polynomial $P_n(s)$ has degree $\deg P_n(s) \le n$, and $Q_n(s)$ is a polynomial part of the series $P_n(s)F(s)$. The solution to this problem always exists with $\deg\ P_n(s) = n$ and $\deg\ Q_n(s) \le n - 1$. The rational function π_n can be represented in a form (5.2), indeed π_n has a partial fraction decomposition of the form

$$\pi_n = \frac{Q_n(s)}{P_n(s)} = \sum_{j=1}^{n} \frac{r_{nj}}{s - z_{nj}}, \tag{5.4}$$

where z_{nj} are zeros of the denominator polynomial $P_n(s)$, and the residues r_{nj} are Christoffel coefficients

$$r_{nj} = \mathrm{res}_{s=z_{nj}}\pi_n(s) = \frac{Q_n(z_{nj})}{P\prime_n(z_{nj})}, \quad j = 1, \ldots, n. \tag{5.5}$$

A similar result can be derived for a more general case, when μ is a matrix-valued measure which corresponds to anisotropic effective properties of the composite [5]. A numerical solution of the problem can be obtained [33,42] solving a constrained optimization problem.

6. Internal variables and waves propagation in viscoelastic media

We consider an application of the Padé approximation of the relaxation spectrum efficiently used in modelling of internal memory variables in the time domain finite-difference simulations of propagation of plane waves through a viscoelastic medium [28–33]. The relation between stress σ and strain ϵ in equation (2.1) governing the waves in a dispersive and dissipative medium is given in the frequency domain by a complex viscoelastic modulus $M(\omega)$ (2.6), $\sigma(\omega) = M(\omega)\epsilon(\omega)$. Taking into account asymptotic behaviour (2.12) of $M(\omega)$ with unrelaxed M_{U} and relaxed M_{R} moduli, and $\delta M = M_{\mathrm{U}} - M_{\mathrm{R}}$, it is convenient to introduce a normalized function $G(\lambda)$ for $\lambda = \mathrm{i}\omega$ as $G(\lambda) = (M_{\mathrm{U}} - M(\lambda/\mathrm{i}))/\delta M$ and rewrite (2.13) for $\lambda \in \mathbb{C} \setminus (-\infty, 0)$ as

$$G(\lambda) = \int_0^\infty \frac{\mathrm{d}\eta(x)}{\lambda + x}. \tag{6.1}$$

The function $G(\lambda)$ is analytic outside the negative real semiaxis in the complex λ-plane, all its singular points are in the interval $(-\infty, 0)$. Padé approximation of order n gives representation of the function $\eta(x)$ as a sum of Heaviside functions, so that

$$\eta(x) \approx \sum_{k=1}^{n} A_k H(x + x_k) \quad \text{and} \quad \mathrm{d}\eta(x) \approx \sum_{k=1}^{n} A_k \delta(x + x_k)\,\mathrm{d}x, \quad x \in [0, \infty). \tag{6.2}$$

The function $\eta(x)$ defined for $x \in [0, \infty)$ is a non-decreasing, non-negative function. Thus, the approximation of the function $G(\lambda)$ is given by

$$G(\lambda) \approx \sum_{k=1}^{n} \frac{A_k}{\lambda - x_k}, \tag{6.3}$$

with x_k being the kth simple pole on the negative real semiaxis with positive residue A_k, and n is the total number of poles. The approximation of the complex modulus $M(\omega)$ is given now by

$$M(\omega) \approx M_{\mathrm{U}} - \delta M \sum_{k=1}^{n} \frac{A_k}{\mathrm{i}\omega - x_k}. \tag{6.4}$$

Equation (6.4) gives a discrete approximation of the complex modulus $M(\omega)$ and represents it as a partial fraction. The real parameters A_k and x_k in this representation contain all the information about the relaxation spectrum of the medium and can be obtained from the parameters of the Padé approximation of the spectral function $F(s)$ discussed in previous section.

Padé approximation of the complex modulus $M(\omega)$ provides a relationship between the stress σ and strain ϵ in the time domain

$$\sigma(t) = M_{\mathrm{U}} \left[\epsilon(t) - \sum_{k=1}^{n} \zeta_k(t) \right]. \tag{6.5}$$

Equation (6.5) represents the stress σ as a sum of the elastic part $M_{\mathrm{U}}\epsilon(t)$ and an anelastic part defined by n internal memory variable functions $\zeta_k(t)$. These internal variables satisfy the system of the first-order differential equations

$$\frac{\mathrm{d}\zeta_k(t)}{\mathrm{d}t} - x_k \zeta_k(t) = M_{\mathrm{U}}^{-1} \delta M A_k \varepsilon(t), \quad k = 1, \ldots, n. \tag{6.6}$$

The coefficients of this system of differential equations can be calculated using the poles and residues of the Padé approximant of the spectral function $F(s)$ discussed in the previous section.

As an example, we consider a wave propagating in a Hashin–Shtrikman composite with the spectral function (4.12). In this example, we assume that the composite is made of the same materials as before with properties $c_0 = 1$ and $c_1(\omega)$, so that $s = 1 + i\omega\tau$. Then, substituting s in (4.13) and using the effective relaxation constant for the composite $\tau_1^* = \tau/(1 - z_0)$ we have a one-pole approximation for $\tilde{G}(\lambda) = G(\lambda)\delta M$

$$\tilde{G}(\lambda) = \frac{m_0/\tau}{\lambda + x_0} \quad \text{and} \quad x_0 = \frac{1}{\tau_1^*}. \tag{6.7}$$

From this, we immediately have the coefficients of the differential equation (6.6) for the evolution of the memory function $\zeta_1(t)$. The number of internal memory functions equals the number of terms in the approximation of the spectral function $F(s)$. So modelling processes in a microstructured medium with the spectral measure μ having n poles requires n internal functions $\zeta_k(t)$. Similar to the one-pole Hashin–Shtrikman composite example, the coefficients of the differential equations governing the evolution of these memory functions $\zeta_k(t)$ can be obtained from the poles and residues of the Padé approximation of the spectral function of the composite.

This approach can be used for modelling and simulation of the waves propagating in the medium that is evolving in time. When the microstructure of the composite changes depending on applied forces, ageing, temperature or other factors, the microstructural changes are reflected in the spectral measure evolving with the microstructure as its moments are determined by the correlation functions (3.13). The evolution of the spectral measure then results in the evolution of the coefficients of the differential equations (6.6) governing the internal variables ζ_k.

7. Conclusion

This paper shows that the parameters of the relaxation function of a composite medium are determined by the spectral measure of the operator $\Gamma\chi$ naturally arising in the problem considered at the microscale. We show that the resonances at the microlevel determine the material's relaxation times and the relaxation spectrum. In application to the modelling of waves propagation through a viscoelastic composite medium, we show that the internal resonances in a composite determine the equations for the evolution of internal memory variables characterizing dispersion and dissipation in wave propagation through the composite material.

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